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Quantum and classical features in the explanation of collisional decoherence

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Abstract. A simple theoretical argument is given in order to explain the quantitative estimate of the effect of collisional decoherence in matter-wave interferometry. The argument highlights the relevance of quantum and classical features in the description of the phenomenon, showing in particular the connection between the formula used for the experimental fit and the loss term in the classical linear Boltzmann equation.

1. Introduction

Paradoxical as it may seem, one of the most intriguing features of the quantum world is certainly its relationship to the classical one [1]. Apart from the conceptual charm, this question is of practical relevance in many respects. A full understanding of this issue would give an answer as to which quantum phenomena might appear or persist on a meso- or macroscopic scale, to the degree of feasibility of quantum computation, to the reliance of classical pictures and classical computations, often simpler and more intuitive. The first significant steps in this direction have been given by recent experiments in which loss of coherence due to the interaction with the environment can be quantitatively studied. This phenomenon goes under the name of decoherence, and its theoretical description is based on an understanding of open system dynamics [2].

In this brief paper we will focus on recent beautiful experiments concerned with the observation of collisional decoherence in matter-wave interferometry [3], sketchily giving a simple theoretical argument for the loss of visibility, thus showing the connection with the classical linear Boltzmann equation and further giving an exact expression for the macroscopic scattering cross-section.

2. Analysis of collisional decoherence

In the aforementioned experiments the visibility of the interference fringes, obtained by letting a beam of fullerenes go through a Talbot-Laue interferometer, is progressively reduced by raising the pressure of the background gas present in the experimental apparatus. The visibility decreases according to the formula

$$V = V_0 \exp(-\Gamma t), \tag{1}$$

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where V_0 is the reference value, t the time of flight through the apparatus, and Γ a decoherence rate given by

$$\Gamma = n v_0 \sigma_{\mathrm{macro}}(v_0), \tag{2}$$

with n the density of the gas, M the mass of the fullerenes, $v_0 = p_0/M$ the modulus of their incoming velocity, supposed to be essentially unchanged despite the collisions with the background particles, $\sigma_{\mathrm{macro}}(v_0)$ the total macroscopic scattering cross-section off the background gas, parametrically depending on the modulus of the incoming velocity or equivalently on momentum. To give a theoretical justification of formula (1) besides a detailed characterization of the experimental apparatus (in this connection see also [4]) one essentially needs a quantum mechanical description of the fullerene dynamics due to collisions with a surrounding gas. This is achieved by means of a quantum master-equation which, as the underlying physics in terms of collisions obviously tells, is actually a quantum counterpart of the classical linear Boltzmann equation. The history of this master-equation is relatively long, and we refer the reader to [5] for a discussion of this point. A general result in this direction, obviously still open to improvements, is given in [6], to which we refer for further details and references. The master-equation takes the form

$$\begin{aligned}\frac{d\hat{\rho}}{dt} &= -\frac{i}{\hbar}[\hat{\mathsf{H}}_0, \hat{\rho}] + \frac{n}{M^2}\int d^3\boldsymbol{q}\, \Sigma(q) \\ &\times \left\{ e^{(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}} \sqrt{S(\boldsymbol{q}, \hat{\mathsf{p}})}\hat{\rho}\sqrt{S(\boldsymbol{q}, \hat{\mathsf{p}})} e^{-(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}} - \frac{1}{2}\left[S(\boldsymbol{q}, \hat{\mathsf{p}}), \hat{\rho}\right]\right\},\end{aligned} \tag{3}$$

with $\hat{\mathsf{x}}$ and $\hat{\mathsf{p}}$ being the position and momentum operators for the test particle (presently the fullerene), $\hat{\mathsf{H}}_0 = \hat{\mathsf{p}}^2/2M$, $\Sigma(q) = M^2(2\pi\hbar)^3(2\pi/\hbar)|\tilde{t}(q)|^2$[$\tilde{t}(q)$ being the Fourier transform of the interaction potential], $S(\boldsymbol{q}, \hat{\mathsf{p}})$ the operator-valued dynamic structure factor, given by the Fourier transform of the time-dependent spatial autocorrelation function of the gas

$$\begin{aligned}S(\boldsymbol{q}, E(\boldsymbol{q}, \boldsymbol{p})) &= \frac{1}{2\pi\hbar}\int dt \int d^3\boldsymbol{x}\, e^{(i/\hbar)[E(\boldsymbol{q},\boldsymbol{p})t - \boldsymbol{q}\cdot\boldsymbol{x}]} \\ &\times \frac{1}{N}\int d^3\boldsymbol{y} \left\langle N(\boldsymbol{y})N(\boldsymbol{x}+\boldsymbol{y}, t)\right\rangle,\end{aligned} \tag{4}$$

with $\boldsymbol{q}$ and $E \equiv E(\boldsymbol{q}, \boldsymbol{p}) = (q^2/2M) + ((\boldsymbol{p}\cdot\boldsymbol{q})/M)$ being the momentum and energy transferred to the fullerene molecule in each single collision. The two-point correlation function $S(\boldsymbol{q}, E)$ is related, as shown by van Hove [7], to the macroscopic differential scattering cross-section of a test particle off a medium through the formula

$$\frac{d^2\sigma_{\mathrm{macro}}}{d\Omega dE} = \frac{p'}{p}\Sigma(q)S(\boldsymbol{q}, E). \tag{5}$$

Equation (3) correctly avoids the extra 2π factor appearing for example in the well-known result of Gallis and Fleming [8], as stressed in [9] and also found in [10], in both of which a particular example of a dynamic structure factor also implicitly appears. The redundancy of this 2π factor can be best understood in physical terms as in [2], where the authors already stressed that this factor would lead to a decoherence rate given by 2π times the total scattering rate. Experiments do in fact rule out this factor. With respect to other results the quantum linear Boltzmann equation (3) encompasses the momentum of the test particle as a dynamical variable, thus allowing for a correct description of energy transfer and for the expected thermal stationary solution [11]. Since on the time scale of the experiment thermalization does not play a role, as a first simplification the operator $\hat{\mathsf{p}}$ in $S(\boldsymbol{q}, \hat{\mathsf{p}})$ can be replaced by $\boldsymbol{p}_0$, the incoming momentum of the fullerene. Equation (3) thus becomes, by exploiting (5),

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{\mathsf{H}}_0, \hat{\rho}] + \frac{n}{M^2}\int d^3\boldsymbol{q}\, \Sigma(q) S(\boldsymbol{q}, \boldsymbol{p}_0) e^{(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}}\hat{\rho} e^{-(i/\hbar)\boldsymbol{q}\cdot\hat{\mathsf{x}}} - n\frac{p_0}{M}\sigma_{\mathrm{macro}}(p_0)\hat{\rho}. \quad (6)$$

Note that the dependence on the incoming momentum of the test particle is still crucial in order to explain the velocity dependence in the macroscopic scattering cross-section appearing in (2). The quantum nature of (6), apart from the free evolution responsible for the interference phenomena, only appears in the second term on the r.h.s., the loss term simply being a multiplicative factor as in the classical linear Boltzmann equation, apart from the obvious fact that the microscopic scattering cross-section describing the single collision is based on a quantum or at least a semi-classical calculation [12]. The second term on the r.h.s. of (6) however does not contribute to the interference fringes, because of its rapid oscillations leading to a destruction of the off-diagonal matrix elements as described e.g. in [13, 2]. Therefore equation (6) predicts an exponential decay of the intensity relevant for the interference fringes according to the rate $n(p_0/M)\sigma_{\mathrm{macro}}(p_0)$, which can be simply calculated from the loss term in the classical linear Boltzmann equation. Following [12], and expressing the scattering cross-section as a function of the incoming velocity, we can write

$$n v_0 \sigma_{\mathrm{macro}}(\boldsymbol{v}_0) = n v_0 \int d^3u\, f_{\mathrm{MB}}(\boldsymbol{u}) \frac{|\boldsymbol{v}_0 - \boldsymbol{u}|}{v_0} \sigma_{\mathrm{micro}}(\boldsymbol{v}_0 - \boldsymbol{u}), \quad (7)$$

where $f_{\mathrm{MB}}(\boldsymbol{u})$ is the thermal Maxwell-Boltzmann distribution of velocities in the background gas. For a microscopic scattering cross-section of the form

$$\sigma_{\mathrm{micro}}(\boldsymbol{v}_0 - \boldsymbol{u}) = K|\boldsymbol{v}_0 - \boldsymbol{u}|^{\alpha}, \quad (8)$$

the integral in (6) can be exactly calculated. Introducing the most probable velocity $v_{\mathrm{mp}} = \sqrt{2/\beta m}$ of gas particles with temperature $1/\beta$ and mass m one has

$$\begin{aligned}\sigma_{\mathrm{macro}}(v_0) &= \frac{K}{v_0}\int d^3u\, u^{\alpha+1} f_{\mathrm{MB}}(\boldsymbol{u} + \boldsymbol{v_0}) \\ &= K \frac{2}{\sqrt{\pi}} \frac{v_{\mathrm{mp}}^{\alpha+2}}{v_0} e^{(v_0/\mathrm{v}_{\mathrm{mp}})^2} \int_0^{+\infty} dt\, t^{\alpha+2} e^{-t^2} \sinh\left(2t\frac{v_0}{v_{\mathrm{mp}}}\right), \end{aligned} \quad (9)$$

and exploiting the result [14]

$$\int_0^{+\infty} dx\, x^{2\mu-1} e^{-x^2} \sinh(\gamma x) = \frac{\gamma}{2}\Gamma\left(\mu + \frac{1}{2}\right) e^{\frac{1}{4}\gamma^2}\, \Phi\left(1-\mu, \frac{3}{2}; -\frac{1}{4}\gamma^2\right),$$

valid for $\mu > -\frac{1}{2}$, with $\Phi(\alpha, \beta; \gamma)$ being the confluent hypergeometric function, one immediately obtains the exact expression

$$\sigma_{\mathrm{macro}}(v_0) = K \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{\alpha}{2} + 2\right) \frac{v_{\mathrm{mp}}^{\alpha+1}}{v_0} \; \Phi\left[-\left(\frac{\alpha}{2} + \frac{1}{2}\right), \frac{3}{2}; -\left(\frac{v_0}{v_{\mathrm{mp}}}\right)^2 \right]. \tag{10}$$

For the case of interest σ_{micro}, calculated on the basis of an isotropic potential $U(r) = -C_6/r^6$, corresponds to the particular choice [3, 15]

$$K = \frac{\left(\pi^6 \frac{3}{8}\right)^{2/5}}{\sin(\pi/5)\; \Gamma\left(\frac{2}{5}\right)} \left(\frac{C_6}{\hbar}\right)^{2/5}, \qquad \alpha = -\frac{2}{5},$$

thus recovering, when considering only the first contributions in the expansion in terms of the small parameter v_0/v_{mp}, the result given in [16]

$$\sigma_{\mathrm{macro}}(p_0) = \frac{\left(\pi^6 \frac{3}{8}\right)^{2/5}}{\sin(\pi/5)\, \Gamma\left(\frac{2}{5}\right)} \left(\frac{C_6}{\hbar}\right)^{2/5} \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{9}{5}\right) \frac{v_{\mathrm{mp}}^{3/5}}{v_0} \left\{ 1 + \frac{1}{5}\left(\frac{v_0}{v_{\mathrm{mp}}}\right)^2 + \mathcal{O}\left[\left(\frac{v_0}{v_{\mathrm{mp}}}\right)^4\right] \right\}.$$

A full theoretical explanation of the observed data, also taking the detailed features of the interferometer into account, has been hinted at in [3, 16] and will appear in a later publication by the same group [17]. The argument presented here, however, gives a remarkably simple explanation of the experimental results by impinging on both quantum and classical aspects. On one hand one needs a truly quantum linear Boltzmann equation in order to understand how the gain term in the equation does not contribute to the interference pattern, due to a suppression of off-diagonal terms, and on the other hand the loss term, which quantitatively describes the reduction of visibility when treated classically, leads to formula (7) used to fit the experimental data. The main difference between the approach presented here and the one outlined in [3, 16] lies in the fact that here we start with a quantum linear Boltzmann equation already containing, through the dynamic structure factor and the dependence on the momentum of the incoming particle, all the information about the macroscopic scattering cross-section relevant for the loss of visibility. When considering a master-equation like the one by Gallis and Fleming, instead, the macroscopic or effective scattering cross-section depending on the velocity of the incoming fullerene has to be introduced as additional information.

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